

Abstract

A method for selecting lead-candidate compounds capable of binding to a receptor biopolymer from a database containing information about atomic types and mode of covalent bonds of compounds by using a computer, comprising a step of selecting candidate compounds from compounds stored in the database based on quantitative, two-dimensional and/or three-dimensional information of one or more query molecules capable of binding to the biopolymer. The query molecules can be obtained by an automatic structure construction method, for example. The lead-candidate compounds capable of binding to the biopolymer can be retrieved rapidly by using an ordinary personal computer or workstation without requiring huge calculation.